Supplementary Material

Summary of Differential Equation Model

Specific details of model development appear in [7] which we summarize here along with parameter choice within the energy intake (EI) model. For simplicity, we refer to the differential equation model of weight change as the Heymsfield model.

1. The rate of energy stored/lost, ES, is modeled by the sum of the change in energy stores from fat free mass and the change in energy stores arising from fat mass. Because glucose/glycogen stores are modeled by a time averaged constant, the change in energy arising from glycogen is zero. Thus,

$$ES = c_l \frac{dFFM}{dt} + c_f \frac{dF}{dt}.$$

2. EI is modeled by a piecewise defined parameter. EI is the variable we solve for in the computational boundary value algorithm. The only restriction on EI is that EI must be larger than EE at zero fat mass. In the cases where EI is smaller than this value, we must consider an entirely different model that simulates the dynamics of starvation.
3. The main variation in the different models appearing in the literature is how the energy expenditures are modeled. For example, Kozusko [18] models energy expenditure as a multiple of resting metabolic rate (RMR) while the Chow-Hall system [19] models energy expenditure as a linear function of fat and fat free mass [19]. The Heymsfield model divides energy expenditure into four distinct terms: E=RMR+PA+SPA+DIT, where PA represents volitional physical activity associated with

recreational sports, SPA represents activity expenditures corresponding to daily living, and DIT is the rate of energy expended in dietary induced thermo genesis.

4. RMR is modeled by the statistically determined Livingston-Kohlstadt equation for RMR [20]. The RMR formula is modeled by an affine function of body mass to a fractional power and age. Metabolic adaptation during weight loss was modeled as a percent difference from predicted by baseline regression equations with a constant value of -2% taken from Martin et al [21]. The value was set to zero in the EI algorithm if weight was observed to increase. The percentage was only applied after the first month to allow for the delay in adaptation. This adjustment reflects the fast and slow effects of early weight loss observed by Forbes [22].
5. DIT is modeled as a direct proportion of intake. Proportionality constants are obtained from Westerterp [23]. The proportionality constant for overfeeding is applied if weight has been observed to increase.
6. The dynamic portion of individual PA is modeled by a direct proportion of body mass. Baseline energy expenditures resulting from PA are estimated by subtracting baseline DIT, baseline RMR, and baseline SPA (determined through benchmark percentages [24]) from baseline TEE. The proportionality constant for the dynamic PA term for each individual subject is derived as the ratio of individual baseline PA and baseline subject weight.
7. SPA is modeled by integrating the equation: $\Delta SPA = s\Delta E$ where s=0.56 (overfeeding) and s=2/3 (underfeeding). The constant, s, was determined through analysis of the overfeeding studies [25,24,26] and underfeeding studies [27,28]. We solve for the constant of integration by applying baseline data. In the EI algorithm, we applied s=2/3 for all cases.

The Heymsfield model differs from other one dimensional models as it is the only one dimensional model that has been validated on individual longitudinal weight change data sets. The Heymsfield model is also the first of any weight change model that was validated using study data that contained criterion participant intake measured through DXA/DLW.

Computational Model for EI

The algorithm is based on the bi-section shooting method (iterative) for numerical solution of a boundary value (limiting dependent condition) problem [29].

1. Subject baseline weight, height, age, gender and target prescribed EI is entered. Measured bi-weekly weights are also entered.
2. We begin with an initial estimate for EI for intake is given as the prescribed intake. A highest possible estimate for intake is also made as 14% above baseline energy expenditures.
3. The differential equation [7] is integrated using the initial estimate for EI.
4. Model predictions of weight at the end of the two week period are compared to measured weight at this time point. If the magnitude of difference is lower than 1.5 kg (determined from the forward model validation mean absolute error estimates), intake is set equal to the estimate and we are done.
5. If the predicted weight is lower than actual weight plus 1.5 kg, then intake was estimated too low. We increase our initial estimate for intake by taking the midpoint from the current estimate to the largest possible EI (14% above baseline energy expenditures).

6. The differential equation is simulated again. If the predicted weight is lower than the actual measured weight, we increase again halfway to the end point as we did before. If it is higher than measured weight, we estimated to high and we lower the estimate by reducing halfway to the left endpoint.
7. We continue in this manner until we converge to the intake that yields a two week body mass within the allotted range of actual body mass. This numerical procedure is referred to as the *bisection method*.
8. We repeat the process for the next two weeks. Instead of beginning at baseline data, we continue along the trajectory already designated by the differential equation.

EI Model Code:

This worksheet applies shooting to determine intake using the Heymsfield Model
We start with baseline information. WA stands for actual final weight:

```
> with(RealDomain): restart; SS:=1933; Gender:=F; W0:=83.8; TEE0:=2551; kcalTarget:=890;
A:=45; H:=166.99; for i from 0 by 2  to 24 do Tf(i):=i*7 end do;      WA(2):=81.3;
     WA(4):=78.3;   WA(6):=76.7;   WA(8):=76.6;   WA(10):=72.5;  WA(12):=74.3;
     WA(14):=72.9;  WA(16):=73.4;  WA(18):=72.6;  WA(20):=71.6;  WA(22):=73.5;
     WA(24):=73.3;
```

Enter Initial Guess for Intakes

```
> for i from 2 by 2 to 24 do Intake(i):=kcalTarget; end do; WA(0):=W0;
```

$$SS := 1933$$

$$Gender := F$$

$$W0 := 83.8$$

$$TEE0 := 2551$$

$$kcalTarget := 890$$

$$A := 45$$

$H := 166.99$

$Tf(0) := 0$

$Tf(2) := 14$

$Tf(4) := 28$

$Tf(6) := 42$

$Tf(8) := 56$

$Tf(10) := 70$

$Tf(12) := 84$

$Tf(14) := 98$

$Tf(16) := 112$

$Tf(18) := 126$

$Tf(20) := 140$

$Tf(22) := 154$

$Tf(24) := 168$

$WA(2) := 81.3$

$WA(4) := 78.3$

$WA(6) := 76.7$

$WA(8) := 76.6$

$WA(10) := 72.5$

$WA(12) := 74.3$

$WA(14) := 72.9$

$WA(16) := 73.4$

$WA(18) := 72.6$

$WA(20) := 71.6$

$WA(22) := 73.5$

$WA(24) := 73.3$

$$Intake(2) := 890$$

$$Intake(4) := 890$$

$$Intake(6) := 890$$

$$Intake(8) := 890$$

$$Intake(10) := 890$$

$$Intake(12) := 890$$

$$Intake(14) := 890$$

$$Intake(16) := 890$$

$$Intake(18) := 890$$

$$Intake(20) := 890$$

$$Intake(22) := 890$$

$$Intake(24) := 890$$

$$WA(0) := 83.8$$

```
>
```

LIVINGSTON KOHLSTADT Now we enter the parameters of the Livingston Kohlstadt BMR formulas. If you are a woman then a1 would be 248, y1 is 5.09 and p is .4356. If you are a man then a1 is 293, p is 0.4330 and y2 = 5.92

```
> if Gender=M then  a1:=293; y1:=5.92; p:=.4330; else a1:=248; y1:=5.09; p:=.4356; end if;
```

$$a1 := 248$$

$$y1 := 5.09$$

$$p := 0.4356$$

ADAPTATION PARAMETERS Now lets enter the adaptation values: a is the percent that RMR has lowered than expected, r is the percent that SPA has changed relative to the change in TEE. It was seen to average around 2/3 of the change in TEE. Adaptation is 0.02 if there is a decrease in intake and 0 if there is an increase. The change to 2% is done linearly in the first month.

```
> for i from 4 by 2 to 24 do if WA(i-2)>WA(i) then  a(i):=0.02 else a(i):=0 end if; end do: adaptation:=piecewise(t<Tf(4),0,t>Tf(4) and t < Tf(6),a(6),t>Tf(6) and t < Tf(8),a(8),t>Tf(8) and t < Tf(10),a(10),t>Tf(10) and t < Tf(12),a(12),t>Tf(12) and t < Tf(14),a(14),t>Tf(14) and t < Tf(16),a(16),t>Tf(16) and t < Tf(18),a(18),t>Tf(18) and t < Tf(20),a(20),t>Tf(20) and t < Tf(22),a(22),a(24));  r:=2/3;e:=1;
```

$$adaptation := \begin{cases} 0 & t < 28 \\ 0.02 & 28 < t \textbf{ and } t < 42 \\ 0.02 & 42 < t \textbf{ and } t < 56 \\ 0.02 & 56 < t \textbf{ and } t < 70 \\ 0 & 70 < t \textbf{ and } t < 84 \\ 0.02 & 84 < t \textbf{ and } t < 98 \\ 0 & 98 < t \textbf{ and } t < 112 \\ 0.02 & 112 < t \textbf{ and } t < 126 \\ 0.02 & 126 < t \textbf{ and } t < 140 \\ 0 & 140 < t \textbf{ and } t < 154 \\ 0.02 & otherwise \end{cases}$$

$$r := \frac{2}{3}$$

$$e := 1$$

RMR AND TEE We now use the initial data to compute the BMR formula and the inital estimate of current intake, current FFM, current PA, and current DIT. We are assuming that the individual is very close to the base equations equilibrium value. Baseline TEE values are found using a regression formula i
n the IOM database. From here we can estimate the calories they are reducing by:

```
> RMR0:=a1*(W0^(p))-y1*(A); RMR:=a1*(W^(p))-y1*(A+t/365); if Gender=M then  TEE2:=-.0971*W0^2+40.853*W0+323.59; else TEE2:=.0278*W0^2+9.2893*W0+1528.90; end if; CalRed:=TEE0-kcalTarget;kcalTarget;
```

$$RMR0 := 1477.88418$$

$$RMR := 248\, W^{0.4356} - 229.05 - 0.0139452054 t$$

$$TEE2 := 2502.56717$$

$$CalRed := 1661$$

$$890$$

BASELINE SPA: SPA is 32.6% of TEE0

```
> SPA0:=.326*TEE0;
>
```

$$SPA0 := 831.62\text{6}$$

DIT: The Contribution to DIT is assumed to be omega% of Total Caloric Intake: beta=1.19 in overfeeding and .95 in underfeeding.

```
> for i from 2 by 2 to 24 do if WA(i-2)>WA(i) then  b(i):=1 else b(i):=1.14 end if; end
do: beta:=piecewise(t<Tf(2),1,t>Tf(2) and t < Tf(4),1, t>Tf(4) and t < Tf(6),b(6),t>Tf(6)
and t < Tf(8),b(8),t>Tf(8) and t < Tf(10),b(10),t>Tf(10) and t < Tf(12),b(12),t>Tf(12)
and t < Tf(14),b(14),t>Tf(14) and t < Tf(16),b(16),t>Tf(16) and t < Tf(18),b(18),t>Tf(18)
and t < Tf(20),b(20),t>Tf(20) and t < Tf(22),b(22),b(24)):

> omega:=beta*(.075); DIT0:=.075*TEE0; DIT:=omega*NI;
```

$$\omega := 0.075 \left(\begin{cases} 1 & t < 14 \\ 1 & 14 < t \textbf{ and } t < 28 \\ 1 & 28 < t \textbf{ and } t < 42 \\ 1 & 42 < t \textbf{ and } t < 56 \\ 1 & 56 < t \textbf{ and } t < 70 \\ 1.14 & 70 < t \textbf{ and } t < 84 \\ 1 & 84 < t \textbf{ and } t < 98 \\ 1.14 & 98 < t \textbf{ and } t < 112 \\ 1 & 112 < t \textbf{ and } t < 126 \\ 1 & 126 < t \textbf{ and } t < 140 \\ 1.14 & 140 < t \textbf{ and } t < 154 \\ 1 & \textit{otherwise} \end{cases} \right)$$

$$DIT0 := 191.32\text{5}$$

$$DIT := 0.075 \left(\begin{cases} 1 & t < 14 \\ 1 & 14 < t \textbf{ and } t < 28 \\ 1 & 28 < t \textbf{ and } t < 42 \\ 1 & 42 < t \textbf{ and } t < 56 \\ 1 & 56 < t \textbf{ and } t < 70 \\ 1.14 & 70 < t \textbf{ and } t < 84 \\ 1 & 84 < t \textbf{ and } t < 98 \\ 1.14 & 98 < t \textbf{ and } t < 112 \\ 1 & 112 < t \textbf{ and } t < 126 \\ 1 & 126 < t \textbf{ and } t < 140 \\ 1.14 & 140 < t \textbf{ and } t < 154 \\ 1 & otherwise \end{cases} \right) NI$$

Baseline PA: The Contribution to initial PA is the remaining portion:

```
> PA0:=piecewise(TEE0-DIT0-RMR0-SPA0>0,TEE0-DIT0-RMR0-SPA0):
>
```

We now use the initial data to find the constant in the PA formula: PA=m*W.

```
> m:=PA0/W0;
```

$$m := 0.598625513$$

```
> PA:=m*W;
```

$$PA := 0.5986255131 W$$

```
>
```

We now need to know how much energy is in 1 kg of muscle mass and 1 kg of fat mass. These parameters are labelled cl and cf respectively.

```
> cl:=1020; cf:=9500;
```

$$cl := 1020$$

$$cf := 9500$$

BASELINE BODY COMPOSITION AND NHANES FFM RELATIONSHIP:

```
> if Gender=M then y:=min(fsolve(W0=x-71.73349+3.5907722*x-0.38273e-1*A+.6555023*H-0.2296e-2*x*A-0.13308e-1*x*H+0.332e-4*x^2*A-0.7195e-1*x^2+0.6841e-3*x^3-0.162e-5*x^4+0.2721e-3*x^2*H-0.187e-5*x^3*H,x=0..100)); else y:=min(fsolve((W0)=-72.055453+2.4837412*x-0.38273e-1*(A)+.6555023*(H)-0.2296e-2*x*(A)-0.13308e-1*x*(H)-0.390627e-1*x^2+0.332e-4*x^2*(A)+3.5*10^(-7)*x^4+0.2291e-3*x^3+0.2721e-3*x^2*H-0.187e-5*x^3*(H)+x,x=0..200)); end if; F0:=y; FFM0:=W0-F0;
```

$$y := 35.6706547$$

$$F0 := 35.6706547$$

$$FFM0 := 48.1293452$$

FFM Function based on NHANES. Height was set at average height in the US for man and woman.

```
> if Gender=M then FFM:=-71.73349+3.5907722*F(t)-0.38273e-1*A+.6555023*H-0.2296e-2*F(t)*A-0.13308e-1*F(t)*H+0.332e-4*F(t)^2*A-0.7195e-1*F(t)^2+0.6841e-3*F(t)^3-0.162e-5*F(t)^4+0.2721e-3*F(t)^2*H-0.187e-5*F(t)^3*H; else FFM:=-72.055453+2.4837412*F(t)-0.38273e-1*A+.6555023*H-0.2296e-2*F(t)*A-0.13308e-1*F(t)*H-0.390627e-1*F(t)^2+0.332e-4*F(t)^2*A+3.5*10^(-7)*F(t)^4+0.2291e-3*F(t)^3+0.2721e-3*F(t)^2*H-0.187e-5*F(t)^3*H; end if;
```

$$FFM := 35.6845911 + 0.15811828 F(t) + 0.007869279 F(t)^2 + 3.500000000 10^{-7} F(t)^4 - 0.0000831713 F(t)^3$$

Set initial interval: L0=target kcal - .10 target kcal and H0=TEE0+.14 TEE0.

```
> L0:=kcalTarget; H0:=TEE0+.14*TEE0;
```

$$L0 := 890$$

$$H0 := 2908.14$$

Initialize Intake

```
> NI:=piecewise(t<Tf(2),Intake(2),
t>Tf(2) and t<Tf(4),Intake(4),t>Tf(4) and t<Tf(6),Intake(6),t>Tf(6) and t < Tf(8),
Intake(8), t>Tf(8) and t < Tf(10),Intake(10),
```

```
t>Tf(10) and t<Tf(12),Intake(12),t>Tf(12) and t<Tf(14),Intake(14),t>Tf(14) and t <
Tf(16),Intake(16), t>Tf(16) and t < Tf(18),Intake(18),t>Tf(18) and
t<Tf(20),Intake(20),t>Tf(20) and t<Tf(22),Intake(22),t>Tf(22) and t < Tf(24), Intake(24),
t>Tf(24) ,2000):
```

The adaptive thermogensis function is AT=((r2/(1-r2)*(BMR+PA+DIT)+C, where C is a constant of integration.
Let's solve for that C first:

```
> Const:=SPA0-2*(RMR0+PA0+DIT0):
```

W=FFM+F(t)

```
> W:=FFM+F(t):
```

Now we enter the SPA function:

```
> G:=2*((1-adaptation)*RMR+DIT+PA)+Const: SPA:=piecewise(G>0,G):
```

Shooting Bisection Method loop

```
> for i from 2 by 2 to 24 do
   ode:=cl*(diff(FFM,t))+cf*diff(F(t),t)=e*(NI-(1-adaptation)*RMR-DIT-PA-SPA):

   ans:= dsolve( {ode, F(0)=F0}, F(t),numeric):

for j from 2 by 2 to 24 do Ff:= subs(ans(Tf(j)), F(t)):
    if Gender=M then FFMf:=-71.73349+3.5907722*Ff-0.38273e-1*A+.6555023*H-0.2296e-2*Ff*A-
0.13308e-1*Ff*H+0.332e-4*Ff^2*A-0.7195e-1*Ff^2+0.6841e-3*Ff^3-0.162e-5*Ff^4+0.2721e-
3*Ff^2*H-0.187e-5*Ff^3*H: else FFMf:=-72.055453+2.4837412*Ff-0.38273e-1*A+.6555023*H-
0.2296e-2*Ff*A-0.13308e-1*Ff*H-0.390627e-1*Ff^2+0.332e-4*Ff^2*A+3.5*10^(-7)*Ff^4+0.2291e-
3*Ff^3+0.2721e-3*Ff^2*H-0.187e-5*Ff^3*H: end if:

    Wf(j):=Ff+FFMf: end do: if i<11 then
if Wf(i)-WA(i)>1.8 then NewIntake(i):=Intake(i)-100; Intake(i):=NewIntake(i); i:=i-2;
elif Wf(i)-WA(i)<-1.8 then NewIntake(i):=Intake(i)+100; Intake(i):=NewIntake(i): i:=i-2;
end if;
if Intake(i+2) <0 then  i:=i+2; Intake(i):=0; end if;elif i>11 and i< 13 then
```

```
if Wf(i)-WA(i)>.5 then NewIntake(i):=Intake(i)-100; Intake(i):=NewIntake(i); i:=i-2; elif
Wf(i)-WA(i)<-.5 then NewIntake(i):=Intake(i)+100; Intake(i):=NewIntake(i): i:=i-2; end
if;
if Intake(i+2) <0 then  i:=i+2; Intake(i):=0; end if; else
if Wf(i)-WA(i)>.1 then NewIntake(i):=Intake(i)-100; Intake(i):=NewIntake(i); i:=i-2; elif
Wf(i)-WA(i)<-.1 then NewIntake(i):=Intake(i)+100; Intake(i):=NewIntake(i): i:=i-2; end
if;
if Intake(i+2) <0 then  i:=i+2; Intake(i):=0; end if; end if:

    NI:=piecewise(t<Tf(2),Intake(2),
t>Tf(2) and t<Tf(4),Intake(4),t>Tf(4) and t<Tf(6),Intake(6),t>Tf(6) and t < Tf(8),
Intake(8), t>Tf(8) and t < Tf(10),Intake(10),
t>Tf(10) and t<Tf(12),Intake(12),t>Tf(12) and t<Tf(14),Intake(14),t>Tf(14) and t <
Tf(16),Intake(16), t>Tf(16) and t < Tf(18),Intake(18),t>Tf(18) and
t<Tf(20),Intake(20),t>Tf(20) and t<Tf(22),Intake(22),t>Tf(22) and t < Tf(24), Intake(24),
t>Tf(24) ,2000):

end do:
>
>
>
>
```

Output Plots:

```
> with(plots):

plot1:=odeplot(ans,[t,(FFM+F(t))],t=0..Tf(24), labels=["days", "kg"],title="Total
Weight",caption=typeset("A plot of total weight Subject  ",SS));

for i from 1 to 12 do Time(i):=Tf(2*i);

Weight(i):=WA(2*i); end do;

points:={seq([Time(i),Weight(i)],i=1..12)};
```

```
p2:=pointplot(points,color = black, symbol=circle, symbolsize=20);display(plot1,p2);
```

$$plot1 := PLOT(\ldots)$$

$$Time(1) := 14$$

$$Weight(1) := 81.3$$

$$Time(2) := 28$$

$$Weight(2) := 78.3$$

$$Time(3) := 42$$

$$Weight(3) := 76.7$$

$$Time(4) := 56$$

$$Weight(4) := 76.6$$

$$Time(5) := 70$$

$$Weight(5) := 72.5$$

$$Time(6) := 84$$

$$Weight(6) := 74.3$$

$$Time(7) := 98$$

$$Weight(7) := 72.9$$

$$Time(8) := 112$$

$$Weight(8) := 73.4$$

$$Time(9) := 126$$

$$Weight(9) := 72.6$$

$$Time(10) := 140$$

$$Weight(10) := 71.6$$

$$Time(11) := 154$$

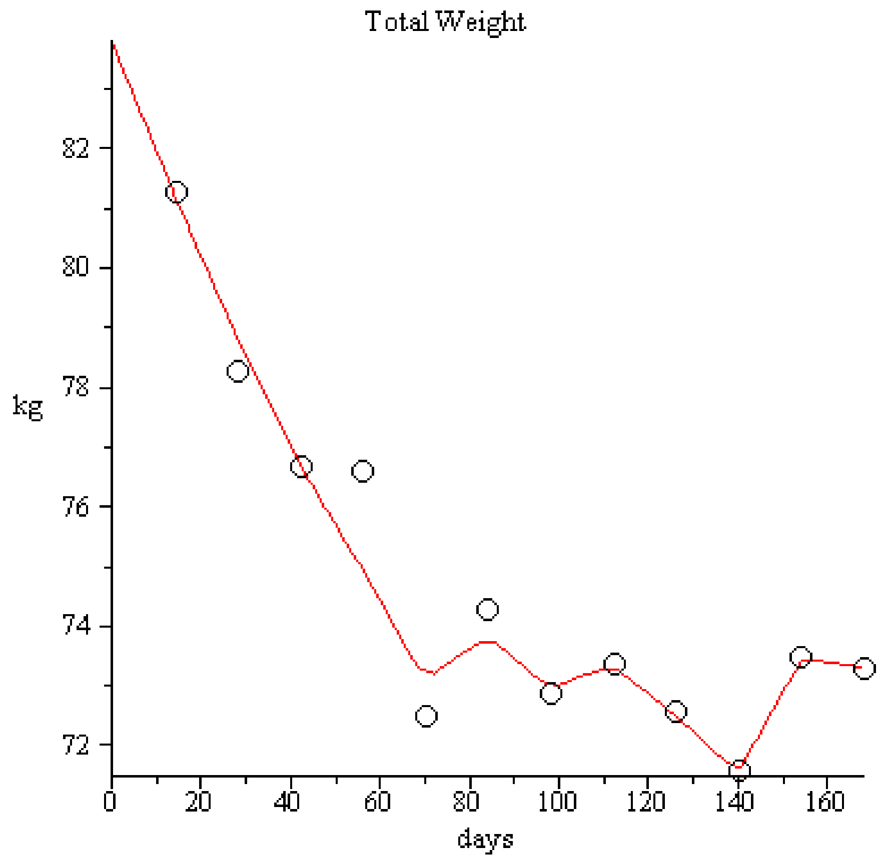
$$Weight(11) := 73.5$$

$$Time(12) := 168$$

$$Weight(12) := 73.3$$

$points := \{[14, 81.3], [28, 78.3], [42, 76.7], [56, 76.6], [70, 72.5], [84, 74.3], [98, 72.9], [112, 73.4], [126, 72.6], [140, 71.6], [154, 73.5], [168, 73.3]\}$

$p2 := PLOT(\ldots)$



A plot of total weight Subject 1933

\> Output EI

```
for i from 2 by 2 to 24 do Intake(i); end do;
```

890

890
890
990
890
2390
1390
2190
1390
1290
2990
1790

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